

5-Methylsalicylic acid
89-56-5 | DTXSID20237472

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.27

Global applicability domain: Inside

Local applicability domain index: 7.15e-01

Confidence level: 6.98e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Hydroxy-3-methylbenzoic acid</div> <div>Measured: 2.86</div> <div>Predicted: 2.26</div>	<div>Image not found</div> <div>5-Methylsalicylic acid</div> <div>Measured: 2.78</div> <div>Predicted: 2.27</div>	<div>Image not found</div> <div>m-Cresotic acid</div> <div>Measured: 2.99</div> <div>Predicted: 2.28</div>
<div>Image not found</div> <div>1,4-Benzenediol, 2,6-dimethyl-</div> <div>Measured: 1.00</div> <div>Predicted: 1.24</div>	<div>Image not found</div> <div>2,3-dimethylhydroquinone</div> <div>Measured: 1.36</div> <div>Predicted: 1.36</div>	